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NUMERICAL TREATMENT OF VERTEX SINGULARITIES AND INTENSITY FACTORS FOR MIXED BOUNDARY VALUE PROBLEMS FOR THE LAPLACE EQUATION IN ${\bf R}^3$

by

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Numerical treatment of vertex singularities and intensity factors for mixed boundary value problems for the Laplace equation in \mathbb{R}^3 .

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<u>Abstract</u>

A numerical method for the computation of the singular behavior of the solution of the Laplace equation is proposed. It is shown that the accuracy of the computed stress intensity factor by the h,p and h-p version of the finite element method has the same order as the square of the error of the solution measured in the energy norm. Numerical examples are given.

1. Introduction

It is well known that the solution of elliptic partial differential equations is singular in the neighborhood of the edges and the vertices of the domain of definition $\Omega \subset \mathbb{R}^3$. The character of the solution can be described by the decomposition of the solution in singular and regular parts (see e.g. [D],[G1], [G2], [K0], [P], [PS1], [PS2]). Singular behavior of the solution is of large importance in many applications. It is, for example, directly related to the problems of fracture mechanics. Hence the numerical determination of the parameters of the singular behavior of the solution is of great interest, for example, in problems of structural mechanics.

The major tool of computational structure mechanics is the finite element method. In the 3 dimensional analysis, one of the most laborious parts of the finite element computation is the mesh generation. Hence the method for the determination of the singular parts of the solution should be fully integrated with the data and algorithm used for solving the boundary value problem of the partial differential generation of interest. In the engineering and mathematical literature, many methods for the computation of stress intensity factors were proposed. Most methods use different approaches for the approximation of the solution, the approximation of singularity functions (and adjoint singularity functions), and the extraction of the intensity factors.

Our analysis addresses the error of the complete approach, i.e., it includes the error of the finite element approximation, the error of the computed singularity function, and the extraction of the vertex intensity factors. The method analyzed here is partially related to the ideas in [LN]. There, however, a different eigenvalue problem was used and no error analysis was performed.

In this paper we propose and analyze such method for the characteristization of the singularity in the neighborhood of the vertex of the domain $\Omega \subset \mathbb{R}$. We restrict ourselves here to the Laplace equation and polyhedral domains only. This paper is the first in a series. The other papers will deal with elasticity problems, which are of especially large interest in engineering. This method was implemented in the program STRIPE [S] and a survey of the results in connection with the analysis of complex airplane structures is given in [A].

In the neighborhood of a vertex the solution u of the boundary value problem can be written in the form (see (2.11))

(1.1)
$$u(x) = u_0(x) + \Sigma C_j S_j(x)$$

where C_j depends (globally) on the solution and $S_j(x)$ depends on the geometry only. The so-called stress intensity functions $S_j(x)$ as well as the so-called stress intensity factors C_j can be computed only numerically. The function u_0 in (1.1) vanishes faster towards the vertex than the functions $S_j(x)$ (see e.g. (2.11b) for exact formulation).

The solution u(x) is computed approximately by the finite element method. The error of the finite element solution u_q satisfies an asymptotic convergence estimate of the form

(1.2)
$$||u_{q} - u|| \le cF(N(q))$$

where $\|\cdot\|$ is typically the energy norm, N(q) is the number of used degrees of freedom and $F(\zeta)$ is a decreasing function depending on the used method, e.g., h, p or h-p version. In practice we usually see in (1.2) approximate equality, i.e. \approx instead \leq . We will show in this paper that the stress intensity factors can be computed with the accuracy $F(N(q))^2$, i.e., denoting by $C_i^{\{q\}}$ the finite element approximation of C_i we get

$$|C_i^{[q]} - C_i| \le C F(N(q))^2$$

where C is independent of q.

This is one of the major results of this paper.

Section 2 gives the formulation of the problem. Section 3 introduces a Steklov problem and shows that the functions S_j in (1.1) are solutions of the problem. In Section 4 we derive a formula for the extraction of the exact stress intensity factors from the exact solution u.

Section 5 elaborates on the finite element method and formulates some assumption about the meshes used. It shows that these assumptions are valid for the standard h, p and h-p versions of the finite element method.

Section 6 elaborates on the numerical computation of the function S_{j} in (1.1) and gives the estimates of the error.

Section 7 describes the numerical computation of the stress intensity factors C_j and proves the error estimate. It shows that the accuracy of $C_j^{[q]}$ is of the same order as the *square of the error* of the finite element solution u_q when measured in the energy norm.

Section 8 presents an illustrative example computed by the p-version of the finite element method implemented in the program STRIPE.

2. Formulation of the problem

Let $\Omega \subset \mathbb{R}$ be a polyhedron with the boundary $\partial \Omega = \bigcup_{\ell=1}^{\ell} \bar{\Gamma}_i = \Gamma$, where Γ_i are the planar (open) faces of $\partial \Omega$. By V_i , $i=0,1,\cdots,m$ we denote the vertices of Ω and will assume that the vertex $V=V_0$ is located in the origin (i.e. $V_0=0$). By E_j , $j=1,2,\cdots,n$ we denote the (open) edges of Ω . \bar{E}_i , $i=\ell,\cdots,n_0$, are all the edges containing the vertex V_0 . Let $\delta=\min\{\mathrm{dist}(E_i,V_0)\}$, $\ell=n_0+1,\cdots,n$. Further by $Q_\rho,\rho>0$ we denote the open ball with the center in V_0 and radius ρ . Set $R=\min\{1,\frac{1}{3},\delta\}$ then obviously $Q_{2R}\cap \Omega=Q_{2R}\cap K$ where K is the infinite cone coinciding with Ω in the neighborhood of V_0 . For any $\rho<\delta$ we denote $\Omega_\rho=Q_\rho\cap\Omega$, $\bar{\Gamma}_\rho^0=\partial Q_\rho\cap\bar{\Omega}$, $\Gamma_\rho=\Gamma\cap\bar{Q}_\rho$. Further let $\Gamma=\Gamma_D\cup\Gamma_N$ where $\Gamma_D=U$ $\bar{\Gamma}_J$ $\Gamma_N=U$ Γ_J , I=0 I=0 I=1 I=

We will be interested in the (weak) solution of the boundary value problem

$$(2.1a) -\Delta u = g in \Omega$$

(2.1b)
$$u = 0$$
 on Γ_D

(2.1c)
$$\frac{\partial u}{\partial n} = g_N$$
 on Γ_N .

Denote by $H^1(\Omega)$ the usual Sobolev space, and let

(2.2a)
$$H_D^1(\Omega) = \{u \in H^1(\Omega) | u = 0 \text{ on } \Gamma_D \} \text{ if } \Gamma_D \neq \phi$$

(2.2b)
$$H_D^1(\Omega) = \{u \in H^1(\Omega) | \int_{\Omega} u \, dx = 0\} \quad \text{if} \quad \Gamma_D = \phi.$$

Further let

$$(2.3) B_{\Omega}(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \nabla \mathbf{u} \cdot \nabla \mathbf{v} \, d\mathbf{x}$$

be the bilinear form defined on $\ H^1_D(\Omega)\times H^1_D(\Omega)$ and

(2.4)
$$\|\mathbf{u}\|_{\mathbf{E}(\Omega)} = (\mathbf{B}_{\Omega}(\mathbf{u}, \mathbf{u}))^{1/2}$$
.

Obviously $\|\cdot\|_{E(\Omega)}$ is equivalent with the standard Sobolev norm $\|\cdot\|_{H^1(\Omega)}$ (if $\Gamma_D \neq \phi$).

Later we will also use the notation

$$\begin{split} &H^1_D(\Omega_\rho) \,=\, \{u\in H^1(\Omega_\rho)\,|\, u\,=\,0\quad \text{on}\quad \Gamma_{\rho,\,D}\} \quad \text{if}\quad \Gamma_{\rho,\,D}\neq \phi\\ &H^1_D(\Omega_\rho) \,=\, \{u\in H^1(\Omega_\rho)\,|\, \int\limits_{\Omega_\rho} u\,\,\mathrm{d}x\,=\,0\} \quad \text{if}\quad \Gamma_{\rho,\,D}=\phi. \end{split}$$

The meaning of $B_{\Omega_{\rho}}(u,v)$ and $\|u\|_{E(\Omega_{\rho})}$ is obvious.

Now the weak formulation of the problem (2.1)-(2.3) is: Find $u \in H^1_D(\Omega)$ such that

(2.5)
$$B_{\Omega}(u,v) = \int_{\Omega} qv \, dx + \int_{\Gamma} g_{N}v \, ds \text{ for all } u \in H^{1}_{D}(\Omega).$$

If $\Gamma_D = \phi$ we assume $\int_{\Omega} g \, dx + \int_{\Gamma} g_N \, ds = 0$.

(By ds we denoted the surface element).

We assume that g and g_n are such that the weak solution exists (and is unique) e.g. $g \in L^{\Omega}(\Omega)$, $g_N \in L^{\Omega}(\Gamma_N)$. Further we will assume that

(2.6)
$$a) \quad g = 0 \quad \text{in } \Omega_{2R}$$

$$b) \quad g_{N} = 0 \quad \text{on } \Gamma_{2R, N}$$

Remark 2.1. We assumed that u=0 on Γ_D for simplicity only. The assumption (2.6) (together with u=0 on $\Gamma_{2R,D}$) is more essential. We will briefly comment on it in Section 7.

Together with the usual cartesian coordinates $x=(x_1,x_2,x_3)$, we also will use in the neighborhood of V_0 (specifically in Ω_ρ) the spherical (polar) coordinate system, (r,θ,φ) centered in the vertex V_0 .

Let $\mathscr{S} = \{S\}$ be the set of all functions $S \in H^1_D(\Omega_R)$ having the form

(2.7)
$$S = r^{\Lambda}w(\theta, \varphi), \quad \Lambda > -\frac{1}{2}$$

and satisfying (in the weak form) the equations

$$(2.8a) -\Delta S = 0 in \Omega_{R}$$

$$(2.8b) S = 0 on \Gamma_{R,D}$$

(2.8c)
$$\frac{\partial S}{\partial n} = 0$$
 on $\Gamma_{R, N}$

In the case when all the faces $\bar{\Gamma}_j$, $j=1,\cdots,n$ which contain V_0 belong to the Neumann part of the boundary (i.e. $\Gamma_{R,D}=\phi$), the constant function also satisfies (2.8) but we do not include it in \mathcal{S} .

Below we will see that the set $\mathscr S$ is not empty and is denumerable, i.e. $\mathscr S=\{S_1,S_2,\cdots\}$ with $S_j=r^{\Lambda j}w_i(\theta,\varphi),\ \Lambda_j\in\mathbb R.$ We will assume that the S_j are ordered such that $\Lambda_j\leq\Lambda_{j+1}$. The functions $S\in\mathscr S$ will be called singularity functions.

Since

$$\frac{\partial S}{\partial r} = \Lambda r^{-1} S$$

the function S satisfies the equation

(2.9)
$$B_{\Omega_{R}}(S, v) = \Lambda b_{R}(S, v) \quad \forall v \in H_{D}^{1}(\Omega_{R})$$

where

(2.10)
$$b_{R}(u,v) = R^{-1} \int_{R}^{0} uv \, ds$$

It is well known (see e.g. [D] [G1],[G2],[K0],[P]) that the solution u of (2.1) (or equivalently (2.5)) admits (under assumption (2.6) for any s>0 the following decomposition on Ω_R :

(2.11a)
$$u = u_0 + \sum_{\Lambda_j + 1/2 \le s} c_j s_j, s_j \in g$$

where

(2.11b)
$$\int_{\Omega_{\mathbf{R}}} |\nabla \mathbf{u}_0|^2 r^{-2s} dv < \infty.$$

Here (2.11b) relates to the seminorm of the weighed Sobolev space $H^1_{-S}(\Omega_R)$. (2.11b) implies that u_0 is in $H^1_{-S}(\Omega_R)$ modulo constants. If $\Gamma_{R,D} \neq \phi$, then $u_0 \in H^1_{-S}(\Omega_R)$.

We will obtain (2.11) as a consequence of the results in Section 3 and 4. Equation (2.11) shows that the behavior of the solution near the vertex is determined by the singularity functions $S_{\mathbf{j}}$. Let

$$w_{s} = \sum_{\Lambda_{j} + \frac{1}{2} \leq s} C_{j} S_{j},$$

then the relative error in the energy norm between u and w goes to zero for $r\longrightarrow 0$, because of (2.11b). Therefore w is a good approximation of u in $H^1(\Omega_R)$ if r is sufficiently small.

The numbers C in (2.11) are called the vertex intensity factors.

With each singularity function S_j of the form (2.7) we will associate the adjoint singularity function

$$(2.12) S_{-,j} = r^{-1-\Lambda_j} w_{,j}(\theta, \varphi)$$

It is easy to check that $S_{-,j}$ satisfies (2.8 abc), but $S_{-,j} \notin H_D^1(\Omega_R)$.

3. The Steklov problem

Coming back to (2.9) we introduce the Steklov eigenvalue problem: Find all pairs (\hat{S}, Λ) , $\hat{S} \in H^1_D(\Omega_R)$ such that (2.9) holds.

In the case that $\Gamma_{R,D} = \phi$, the trivial function $\hat{S} = 1$, $(\Lambda = 0)$ will not be considered here.

We can cast the Steklov problem in a different form. To this end define the operator $T:H^1_D(\Omega_R)\longrightarrow H^1_D(\Omega_R)$ such that (with (2.10))

(3.1)
$$B_{\Omega_{R}}(Tu, v) = b_{R}(u, v) \quad \forall u, v \in H_{D}^{1}(\Omega_{R})$$

The operator T is obviously selfadjoint and is well defined by the coercivity of B_{Ω_R} . Since the trace mapping $u \longmapsto u|_{\Gamma_R^o}$, $H^1(\Omega_R) \longrightarrow L^2(\Gamma_R^0)$, is compact and the bilinear form $b_R(u,v)$ is continuous on $L^2(\Gamma_R^0) \times L^2(\Gamma^0)$, the operator $T: H^1_D(\Omega_R) \longrightarrow H^1_D(\Omega_R)$ is compact.

Now the Steklov problem (2.9) can be cast in the following form: Find (\hat{S},Λ) , $\hat{S}\in H^1_D(\Omega_R)$ such that

$$(3.2) \qquad \qquad \hat{ATS} = \hat{S}$$

or denoting $\lambda = \frac{1}{\Lambda}$

It is known from the theory of compact selfadjoint linear operators that there are countably many eigenpairs (\hat{S}_j, λ_j) , $\lambda_j \in \mathbb{R}$, with no accumulation points except at $\lambda = 0$. Furthermore the eigenfunctions S_j yield an orthonormal basis of the closure of the range of T. If λ_j is a simple eigenvalue, then S_j is uniquely defined up to a multiplicative factor. For multiple eigenvalues $\lambda_j = \ldots \lambda_{j+m}$ we will assume that S_j, \cdots, S_{j+m} are orthonormal with respect to B_{Ω_R} . In this case only the span $\{S_j, \cdots, S_{j+m}\}$ is

. unique but the orthogonal basis $\{S_j,\cdots,S_{j+m}\}$ is not unique.

From (3.1) we readily see that for u = Tv we have

(3.3a)
$$\Delta u = 0 \quad \text{in} \quad \Omega_{R}$$

$$(3.3b) u = 0 on \Gamma_{R,D}$$

(3.3c)
$$\frac{\partial u}{\partial n} = 0 \quad \text{on} \quad \Gamma_{R, N}$$

(3.3d)
$$\frac{\partial u}{\partial n} = v \quad \text{on} \quad \Gamma_{R}^{0}.$$

Hence the eigenfunctions \hat{S}_j form a Hilbert space basis of the space (defined in the variational sense):

$$\mathcal{Z}(\Omega_{R}) \ = \ \{u \in H^{1}_{D}(\Omega_{R}), \ \Delta u \ = \ 0 \quad \text{in} \quad \Omega_{R}, \ u \ = \ 0 \quad \text{on} \quad \Gamma_{R,\,D}, \frac{\partial u}{\partial n} \ = \ 0 \quad \text{on} \quad \Gamma_{R,\,N}\} \,.$$

We also see that functions $\hat{S}_j|_{\Gamma_R^o}$ form an orthogonal basis of the space $L^2(\Gamma_R^0)$.

As usually we will assume that

$$(3.4a) B_{\Omega_{R}}(\hat{S}_{j}, \hat{S}_{k}) = \begin{cases} 0 & \text{for } k \neq j \\ 1 & \text{for } k = j \end{cases}$$

and

$$(3.4b) \qquad b_{R}(\hat{S}_{j}, \hat{S}_{k}) = \begin{cases} 0 & \text{for } k \neq j \\ \frac{1}{\bar{\Lambda}_{j}} = \lambda_{j} & \text{for } k = j \end{cases}.$$

In the case that $\Gamma_{R,D} = \phi$, we will understand $L(\Omega_R)$ and $L^2(\Gamma_R^0)$ as spaces modulo constants.

So far we assumed that $H^1_D(\Omega_R)$ is a real space. We will extend it to the complex space C by defining, as usual,

$$B_{\Omega_{R}}(u,v) = \int_{\Omega_{R}} (\nabla u) \cdot \overline{(\nabla v)} dx,$$

with $b_{r}(u,v)$ being analogously defined.

Denote by $\rho(T)$ the resolvent set of T, i.e. $\rho(T) = \{z | z \in \mathbb{C}, (zI-T)^{-1}\}$ exists as a bounded operator on $H^1_D(\Omega_R)$ (by I we denoted the identity operator). Further let $\sigma(T)$ be the spectrum of T i.e. $\sigma(T) = \mathbb{C} - \rho(T)$. For any $z \in \rho(T)$ denote $R_z(T) = (zI-T)^{-1}$, the resolvent operator.

Let μ be a nonzero eigenvalue of T with multiplicity m+1 and γ be a circle in C centered at μ which lies in $\rho(T)$ and which encloses no other point of $\sigma(T)$ than μ . Then the spectral projection associated with T at μ is defined

(3.5)
$$E = E(\mu) = \frac{1}{2\pi i} \int_{\gamma} R_{z}(T) dz$$

see e.g. [BO1]. Now we prove

Theorem 3.1 Let (\hat{S}_k, Λ_k) be a Steklov eigenpair. Then \hat{S}_k has the form $\hat{S}_k(r, \theta, \varphi) = r w_k(\theta, \varphi)$

<u>Proof</u> Let $\hat{S}_{k}(r,\theta,\phi)$ be the Steklov eigenfunction. Then we can, for any $0 < r \le R$, define

(3.7)
$$a_{j}^{(k)}(r) = \int_{\Gamma_{r}} \hat{S}_{k}(r,\theta,\varphi) \hat{S}_{j}(R,\theta,\varphi) ds$$

For $0 < r_1 < R$ apply now Green's formula for $\hat{S}_k(r,\theta,\phi)$ and $\hat{S}_j(\frac{R}{r_1}r,\theta,\phi)$ in Ω_{R_1} . Then it can be readily seen that

(3.8)
$$B_{\Omega_{R_1}}(\hat{s}_k(r,\theta,\varphi), \hat{s}_j(\frac{rR}{r_1},\theta,\varphi))$$

$$= \int_{\Gamma_{r_1}^0} \frac{\partial \hat{s}_k}{\partial r} (r,\theta,\varphi), \hat{s}_j(R,\theta,\varphi) ds.$$

On the other hand we have by scaling (2.9)

$$(3.9) \qquad \qquad \mathsf{B}_{\Omega_{\mathsf{R}_{1}}}(\hat{\mathsf{S}}_{\mathsf{k}}(\mathsf{r},\theta,\varphi),\ \hat{\mathsf{S}}_{\mathsf{j}}(\frac{\mathsf{r}_{\mathsf{R}}}{\mathsf{r}_{\mathsf{1}}},\theta,\varphi))$$

$$= \Lambda_{\mathsf{j}} \ \mathsf{r}_{\mathsf{1}}^{-1} \int_{\Gamma_{\mathsf{k}}} \hat{\mathsf{S}}_{\mathsf{k}} \ (\mathsf{r}_{\mathsf{1}},\theta,\varphi),\ \hat{\mathsf{S}}_{\mathsf{j}}(\mathsf{R},\theta,\varphi) d\mathsf{s}$$

$$= \mathsf{a}_{\mathsf{j}}^{(\mathsf{k})}(\mathsf{r}_{\mathsf{1}}) \Lambda_{\mathsf{j}} \mathsf{r}_{\mathsf{1}}^{-1}.$$

Further we see that

(3.10)
$$\int \frac{\partial \hat{S}_{k}}{\partial r} (r_{1}, \theta, \varphi), \ \hat{S}_{j}(R, \theta, \varphi) ds.$$

$$= \frac{da_{j}^{(k)}}{dr} (r_{1})$$

where the derivative on the right hand side of (3.10) is understood in the weak (distributional) sense. Combining now (3.7)-(3.10) we get

$$\frac{da_{j}^{(k)}}{dr} = \Lambda_{j}r^{-1}$$

and hence

(3.11)
$$a_{j}^{(k)}(r) = C_{j}^{(k)} r^{\Lambda_{j}}, \ 0 < r \le R$$
.

From (3.4b) we get $C_j^{(k)} = 0$ for $k \neq j$. Since $\hat{S}_j|_{\Gamma_R^0}$ is a basis of $L^2(\Gamma_R^0)$ we obtain

$$\hat{S}_{k}(\mathbf{r}, \theta, \varphi) = \frac{1}{R^{\Lambda_{k}}} r^{\Lambda_{k}} \hat{S}_{k}(\mathbf{R}, \theta, \varphi) =: r^{\Lambda_{k}} w_{k}(\theta, \varphi)$$

which was to be proven.

We get immediately

4. The vertex intensity factors

Let u be the solution of the boundary value problem (2.1) (or equivalently (2.5)) and assume that (2.6) holds. Then we have $u|_{\Omega_R} \in \mathcal{L}(\Omega_R)$ and hence by corollary 3.2 u can be written in the terms of the basis functions $\{S_1, S_2, \ldots\}$

$$(4.1) u = \sum_{j=1}^{\infty} \tilde{C}_{j} S_{j}.$$

Let us show that (4.1) implies the decomposition (2.11) with $C_j = \tilde{C}_j$. Let

$$u_0 = u - \sum_{\Lambda_j + \frac{1}{2} \le s} \tilde{c}_j s_j = \sum_{\Lambda_j + \frac{1}{2} > s} \tilde{c}_j s_j$$

and for $0 < \rho \le R$

$$F(\rho) := \int_{\Omega_{\rho}} |\nabla u_0|^2 dx,$$

then by the orthonormality of S_i we get

$$F(R) = \sum_{\Lambda_{j} + \frac{1}{2} > s} \tilde{C}_{j}^{2} = C < \infty.$$

Further let

$$\widetilde{\mathbf{u}}_{0}(\mathbf{x}) = \mathbf{u}_{0}\left[\stackrel{\varrho}{\mathbf{R}}\mathbf{x}\right] = \sum_{\mathbf{\Lambda}_{j} + \frac{1}{2} > \mathbf{s}} \widetilde{\mathbf{C}}_{j}\left[\stackrel{\varrho}{\mathbf{R}}\right]^{\mathbf{\Lambda}_{j}} \mathbf{s}_{j};$$

then for sufficiently small $\varepsilon > 0$

$$F(\rho) = \frac{\varrho}{R} B_{\Omega_{R}}(\tilde{u}_{0}, \tilde{u}_{0})$$

$$= \frac{\varrho}{R} \sum_{\Lambda_{1} + \frac{1}{2} > s} \tilde{C}_{j}^{2} \left[\frac{\varrho}{R}\right]^{2\Lambda_{j}} \leq \left[\frac{\varrho}{R}\right]^{1 + 2(s - 1/2) + \varepsilon} \sum_{\Lambda_{1} + \frac{1}{2} > s} \tilde{C}_{j}^{2} \leq \bar{c} \rho^{2s + \varepsilon}.$$

Let

$$G = \int_{0}^{R} \int_{\omega \in \Gamma_{R}^{0}} r^{-2s} |\nabla u_{0}|^{2} r^{2} dr d\omega$$

where $d\omega$ denotes the surface element on $\Gamma_{R}^{0}.$ Hence integrating by parts we get

$$G = R^{-2} \int_{0}^{R} r^{-2s} F'(r) dr = R^{-2-2s} F(R) + 2sR^{-2} \int_{0}^{R} r^{-2s-1} F(r) dr$$

and using (4.3) yields

$$\int_{\Omega_{R}} r^{-2s} |\nabla u_{0}|^{2} dx = R^{-2}G = R^{-2-2s}F(R) + 2sR^{-2} \int_{0}^{R} r^{-2s-1}F(r) dr$$

$$\leq \bar{C}(1 + 2s \int_{0}^{R} r^{-1+\varepsilon} dr) \leq C.$$

Therefore (2.11b) holds with $\tilde{C}_j = C_j$. Hence we can use (4.1) and (3.4) to express the intensity factors C_j

$$(4.4) C_{j} = B_{\Omega_{R}}(u,S_{j}) = \Lambda_{j}b_{R}(u,S_{j}) = \frac{\Lambda_{j}}{R} \int_{\Gamma_{R}^{o}} u S_{j}ds.$$

Replacing u, S_j, Λ_j by their finite element approximations, we will use (4.4) in section 7 to compute C_i numerically.

Remark 4.1 Note that in the case when Λ_j is a multiple eigenvalue the functions S_j are not unique and hence C_j depends on the choice of the singularity function S_j . For a simple eigenvalue Λ_j the eigenfunction S_j is unique up to a factor of -1.

5. Finite Element method

Let $\mathcal{P}_q(\Omega), q=1,2,\cdots$ be the partition of Ω into the set of open elements $\mathcal{T}_0^q, i=1,2,\cdots$ $M(q), W_q(\Omega) \in H^1_D(\Omega)$ be the associated finite element C_0 -spaces and let N(q) be the dimension of $W_q(\Omega)$. Further let $M_q=(\mathcal{P}_q(\Omega),W_q(\Omega))$ and $M=\{M_q\}$.

Denoting by $\mathbf{u}_{\mathbf{q}}$ the finite element solution of the problem (2.1) satisfying

$$(5.1) B_{\Omega}(u_{\sigma}, v) = B_{\Omega}(u, v) \ \forall v \in W_{\sigma}(\Omega)$$

we obviously have

$$\|\mathbf{u} - \mathbf{u}_q\|_{\mathbf{E}(\Omega)} = \inf_{\zeta \in \mathbf{W}_q(\Omega)} \|\mathbf{u} - \zeta\|_{\mathbf{E}(\Omega)},$$

where B(u,v) and $\|\cdot\|_{E(\Omega)}$ were defined in Section 2 (see (2.3), (2.4)). If the data g,g_N in (2.1) are sufficiently smooth say $g\in H^{-1+s}(\Omega)$, $g_N=\frac{\partial}{\partial n}G|_{\Gamma_N}$ for some $G\in H^{1+s}(\Omega)$, s>0 then the weak solution $H\in H^1_D(\Omega)$ of (2.1) (resp.(2.5)) exists and is unique. It belongs to $H^{1+s}(\Omega)$ where $\Omega=\Omega-\frac{n}{U}E_J^A$, E_J^A being the Δ neighborhood of E_J^A . In the neighborhood of E_J^A , E_J^A being the Δ neighborhood of E_J^A . In the neighborhood of E_J^A , E_J^A being the E_J^A neighborhood of E_J^A . In the neighborhood of E_J^A , E_J^A being the E_J^A neighborhood of E_J^A . In the neighborhood of E_J^A , E_J^A being the E_J^A point E_J^A and E_J^A being the E_J^A neighborhood of E_J^A . In the neighborhood of E_J^A being the E_J^A being the

(5.3)
$$\|\mathbf{u} - \mathbf{u}_{\mathbf{q}}\|_{\mathbf{E}(\Omega)} = \inf_{\zeta \in \Omega_{\mathbf{q}}(\Omega)} \|\mathbf{u} - \zeta\|_{\mathbf{E}(\Omega)} \le CF(N(\mathbf{q}))$$

Remark 5.1: Later we will assume that an estimate of the form (5.3) with the same function F also holds for a class of solutions which will be specified in Assumptions A_1 , A_2 , A_3 below. It may be that the function F which satisfies Assumptions A_1 , A_2 , A_3 gives a less than optimal error estimate in (5.3), e.g., in the exceptional case when the solution u is smooth.

An interesting question is the characterization of all functions u satisfying (5.3) for a given function F(N(q)) and a given sequence of meshes. For the description of such class of functions in a particular case we refer to [BKP]. In practice we can assume that $\|u-u_q\|_{E(\Omega)} \approx CF(N(q))$ which is a typical case, but in the sequel we will only assume that (5.3) holds.

Let us describe the convergence function F for some typical examples.

Example 5.1. The h-version method on a quasiuniform mesh. Let $P_q(\Omega)$ be the standard family of quasiuniform simplical (in general, curved) meshes of the size $\frac{1}{q}$ (see e.g. [C1],[C2]). Let $W_q(\Omega_R)$ be the set of functions $H^1_D(\Omega)$ which are polynomials, of total degree $\leq d$ on each simplex. Then we have

(5.4)
$$F(N(q)) = N(q)^{-\beta/3}$$

where

(5.5)
$$\beta = \min(d, s, \sigma - \varepsilon), \varepsilon > 0$$
 arbitrary

(5.6)
$$\sigma = \min \left\{ \Lambda_1^{(k)} + \frac{1}{2}, \nu_1^{(\ell)} | k = 0, \dots, m, \ell = 1, 2, \dots, n \right\}$$

where $\Lambda_1^{(k)}$ is the smallest vertex singularly exponent for the vertex singularity function (see (2.11)) and $\nu_1^{(\ell)} = \frac{\pi}{\omega^{(\ell)}}$ where $\omega^{(\ell)}$ is the internal angle of Ω at the edge $\bar{\Gamma}_{\ell}$. If $E_{\ell} = \bar{\Gamma}_{i} \cap \bar{\Gamma}_{j}$ and $i \in D$, $j \in N$ or $i \in N$, $j \in D$ (i.e. the Dirichlet condition is prescribed on one side and Neumann condition on the other side of E_{ℓ}) then $\nu_1^{(\ell)} = \frac{\pi}{2\omega^{(\ell)}}$, instead. By

the regularity theory, we have then $u \in H^{1+\sigma-\epsilon}(\Omega)$, $\epsilon < 0$ arbitrary where we denoted by $H^{1+\sigma-\epsilon}(\Omega)$ the standard Sobolev space with fractional derivatives (for definition see e.g [BL]). (5.4) then follows from the standard theory of the finite element method.

Example 5.2. The p-version of the finite element method. Here $P_q(\Omega)$ is fixed mesh of simplices (generally curved) and $W_q(\Omega)$ is the space of all functions in $H^1_D(\Omega)$ which are polynomials of degree q on each simplex. Then we have

(5.7)
$$F(N(q)) = N^{-(\beta-\epsilon)/3}, \ \epsilon > 0 \ \text{arbitrary}$$

where

$$\beta = \min(s, 2\sigma),$$

where σ is given in (5.6) (see [D1], [D2]).

Example 5.3. The h-p version of the finite element method. Here $P_q(\Omega)$ is sequence of properly selected meshes and $W_q(\Omega)$ is the space of functions in $H^1_D(\Omega)$ which are polynomials of degree R(q) with $R(q) \longrightarrow \infty$ as $q \longrightarrow \infty$ properly selected. We assume that g is an analytic function on Ω and g_N is an analytic function on every face $\overline{\Gamma}_\Omega$. We can then expect that

(5.9)
$$F(N(q)) = e^{-\gamma N^{1/4}}$$

(5.9) was proven in the case that $\Omega \subset \mathbb{R}^n$, n = 1,2 when

$$F(N(q)) = e^{-\gamma N^{1/(n+1)}}$$

see [BG], [GP].

We need now to make additional assumptions about the family M.

 $\underline{A_1}\colon \ \Gamma_R^0$ coincides with the boundaries of the elements \mathcal{I}_i^q of the partition $P_{\sigma}(\Omega).$

(5.10)
$$\inf_{\zeta \in W_{\underline{q}}(\Omega)} \|\mathbf{u} - \zeta\|_{\underline{E}(\Omega)} \leq CF(N(q))$$

 $\underline{A_3}$: Let $u \in \mathcal{L}(\Omega_{2R})$ (as defined in Section 3). Then

(5.11)
$$\inf_{\zeta \in W_{\underline{q}}(\Omega_{\underline{R}})} \|u - \zeta\|_{\underline{E}(\Omega_{\underline{R}})} \leq CF(N(q)).$$

In (5.10) and (5.11) the function F(N(q)) is assumed to be the same as in (5.3).

Let us now discuss the validity of the assumptions A_1 , A_2 , A_3 .

- i) Assumption A_1 : It can be satisfied by the standard finite element technique using the binding mapping of the master element (for the h-p version see [BG] for details).
- ii) Assumption A_3 : Here $u \in \mathcal{L}(\Omega_{2R})$ implies that the function u has only a vertex singularity at $V_0 = 0$ and the edge singularities at the edges $E_i, i=1, \cdots, n_0$, but it has no additional singularities at $\partial \Gamma_R^0$. Therefore, the assumption A_3 is satisfied in the examples 5.1, 5.2 and 5.3 by the direct application of the corresponding approximation results.
- iii) Assumption A_2 : We will briefly sketch its validity for the examples mentioned above.

Example 5.1. The h-version on the uniform mesh. For simplicity we will restrict ourself to the case d = 1. Consider the space

$$\begin{split} \mathcal{H}_2 &= \left\{\mathbf{u} \in H_D^1(\Omega) \, | \, \mathbf{u} \, |_{\Omega_R} \in H^2(\Omega_R) \,, \quad \mathbf{u} \, |_{\Omega - \Omega_R} \in H^2(\Omega - \Omega_R) \right\}, \\ & \left\| \mathbf{u} \right\|^2 &= \left\| \mathbf{u} \right\|^2_{H^2(\Omega_R)} \,\, + \, \left\| \mathbf{u} \right\|^2_{H^2(\Omega - \Omega_R)} \,. \end{split}$$

Further let Π_h be the energy projection operator of H^1_D on $W_q(\Omega)$. Then by the standard approach, see e.g [C1], [C2], we have for $v \in \mathcal{H}_2$.

$$\|\mathbf{v} - \mathbf{\Pi}_{\mathbf{h}} \mathbf{v}\|_{\mathbf{E}(\Omega)} \le \mathbf{Ch} \|\mathbf{v}\|_{\mathcal{H}_{2}(\Omega)}.$$

Applying the interpolation theory (see e.g. [BL]) we see that for 1 < s < 2, $\theta = s-1$

$$\mathcal{H}_{s} = \left\{ \mathbf{H}_{D}^{1}, \mathcal{H}_{2} \right\}_{2, \theta} = \left\{ \mathbf{u} \in \mathbf{H}_{D}^{1}(\Omega) \mid \mathbf{u} \mid_{\Omega_{R}} \in \mathbf{H}^{s}(\Omega_{R}), \mathbf{u} \mid_{\Omega - \Omega_{R}} \in \mathbf{H}^{s}(\Omega - \Omega_{R}) \right\},$$

and hence for any $u \in \mathcal{H}_{S}$,

$$\|\mathbf{u} - \mathbf{\Pi}_{\mathbf{h}}\mathbf{u}\|_{\mathbf{E}(\Omega)} \le \mathbf{Ch}^{\mathbf{S}} \|\mathbf{u}\|_{\mathcal{H}_{\mathbf{S}}}$$

Assume now that u satisfies assumption A_2 . Then u has the same type of singularities in Ω_R and $\Omega - \Omega_R$ as solutions of (2.1) with smooth g and g_N . Hence $u|_{\Omega_R} \in H^{1+\sigma-\epsilon}(\Omega_R)$, $u|_{\Omega - \Omega_R} \in H^{1+\sigma-\epsilon}(\Omega - \Omega_R)$ with σ as in (5.6) and (5.10) follows.

Example 5.2. The p-version. Here the validity of A₂ follows by applying Dorr's results. (see [D1], [D2]). He approximates first the solution u having singularity of the vertex and edge type element by element using weighted (Legendre type) spaces, imposing continuity at the vertices of elements. Then the difference of the approximation on the edges and faces of the neighboring elements (the discrepancy) in the (Legendre) weighted spaces norm is estimated. Then it is shown that it is possible to extend this discrepancy into the elements where the extension mapping is continuous from

the weighted spaces on the boundary to H¹ in the element. Hence only the smoothness of the solution in each element is employed. Realizing that in every element, the function u can be decomposed into a smooth function and the singular functions the arguments of [D1] and [D2] apply.

Example 5.3 The h-p version in \mathbb{R}^2 . Here the singularity is only in the vertices of the domain and there are only finite number of elements which have boundary on Γ_R^0 . As in [BG] we approximate u separately on every element and then remove the discrepancy (discontinuity) of the approximation on the boundary of elements. Because the solution in every (closed) element which nonempty intersection with Γ_R^0 is analytic, the arguments used in [BG] are immediately applicable.

6. Computation of the Singularity Functions

The singularity functions S_j (see Corollary 3.2) will be computed by the finite element method as the approximate eigenfunctions of the Steklov eigenvalue problem. We will assume that the assumptions A_1-A_3 introduced in the section 5 hold.

The finite element solution of the Steklov problem is based on the variational formulation (2.9) (2.10): Find $S_j^{[q]} \in W_q(\Omega_R)$ and $\Lambda^{[q]} \in \mathbb{R}$ such that

$$(6.1) B_{\Omega_R}(S^{[q]}, v) = \Lambda_j^{[q]} b_R(S^{[q]}, v), \forall v \in W_q(\Omega_R).$$

By normalizing the eigenfunctions and orthogonalizing the eigenfunctions for multiple eigenvalues, we have, analogous to (3.4 ab),

(6.2a)
$$B_{\Omega_{\mathbf{R}}}(S_{\mathbf{j}}^{[q]}, S_{\mathbf{k}}^{[q]}) = \begin{cases} 0 & \text{for } \mathbf{k} \neq \mathbf{j} \\ 1 & \text{for } \mathbf{k} = \mathbf{j} \end{cases}$$

(6.2b)
$$b_{\Omega_{R}}(S_{j}^{[q]}, S_{k}^{[q]}) = \begin{cases} 0 & \text{for } k \neq j \\ \frac{1}{\Lambda_{j}^{q}} & \text{for } k = j \end{cases}.$$

Let further (S_j, Λ_j) $j = 1, 2, \cdots$ be the exact eigenpairs. Then we have (sec [BO1]).

Theorem 6.1. Let $S_j, S_{j+1}, \cdots, S_{j+m}$ be the eigenfunctions associated to the eigenvalue Λ_j with multiplicity m+1 (i.e. $\Lambda_j = \Lambda_{j+1} = \dots = \Lambda_{j+m}$). Then for q sufficiently large there exist exact eigenfunction $S_{j+\ell, q}, \ell = 0, \cdots$ (depending on q) and satisfying (3.4) such that

(6.3)
$$\|S_{j+\ell,q} - S_{j+\ell}^{[q]}\|_{E(\Omega_{p})} \le C\varepsilon_{j}$$

$$|\Lambda_{j+\ell} - \Lambda_{j+\ell}^{[q]}| \le C\varepsilon_{j}^{2}$$

where

(6.5)
$$\epsilon_{j} = \sup_{S \in M(\Lambda_{j})} \inf_{\|S\|_{E(\Omega_{R})} = 1} \|S - \zeta\|_{E(\Omega_{R})}$$
$$\zeta \in W_{\alpha}(\Omega_{R})$$

and $M(\Lambda_j)$ is the eigenspace associated to the eigenvalue Λ_j of multiplicity m+1. \square

We will show later that we can impose additional conditions on $S_{j+\ell,q}$. The constant C in (6.3) (6.4) is independent of q but depends on various other factors (see [BO2] for the discussion). In the sequel we will also write S_j instead of $S_{j,q}$ if no misunderstanding occurs.

With the assumption A_2 we get

(6.6)
$$\varepsilon_{j} \leq C_{j} F(N(q))$$

and hence from the theorem 6.1 we get

(6.7)
$$\|S_{j} - S_{j}^{[q]}\|_{E(\Omega_{p})} \le CF(N(q))$$

(6.8)
$$|\Lambda_{j} - \Lambda_{j}^{[q]}| \le C(F(N(q)))^{2}$$

Remark 6.1 Note that the bilinear form $b_k(u,v)$ in (2.10) depends only on u and v on Γ_R^0 . This allows us in practice to eliminate first all unknowns inside Ω_R and obtain an eigenvalue problem on Γ_R^0 only. By proper orderings of unknowns the LU decomposition of the stiffness matrix on Ω_R can be used in the computation of u_q i.e. for the computations of the finite element solution of (2.1).

Let us now write the finite element solution of the Steklov eigenvalue problem in a different way, which is the basis of the estimates (6.3) (6.4). This will be used in the next section too.

Let Π_q^R be the elliptic projection of $H_D^2(\Omega_R)$ into $W_q(\Omega_R)$ defined

bу

$$(6.9) \qquad \qquad \mathsf{B}_{\Omega_{\mathsf{R}}}(\boldsymbol{\Pi}_{\mathsf{q}}^{\mathsf{R}}\mathsf{u},\mathsf{v}) \; = \; \mathsf{B}_{\Omega_{\mathsf{R}}}(\mathsf{u},\mathsf{v}), \forall \mathsf{u} \in \mathsf{H}_{\mathsf{D}}^{1}(\Omega_{\mathsf{R}}), \mathsf{v} \in \mathsf{W}_{\mathsf{q}}(\Omega_{\mathsf{R}}).$$

Define now $T_q = \Pi_q^R T$ where T is given in (3.1). Then T_q converges to T in the norm of linear mappings $H^1(\Omega_R) \longrightarrow H^1(\Omega_R)$ as $q \longrightarrow \infty$.

Further consider the spectral projection $E(\Lambda_j^{-1})$ onto the eigenspace of Λ_j^{-1} of T given by (3.5) where γ is a circle which encloses Λ_j^{-1} but no Λ_k^{-1} which $\Lambda_k \neq \Lambda_j$:

(6.10)
$$E(\Lambda_{j}^{-1}) = \frac{1}{2\pi} \int_{\gamma} (T - z\Gamma)^{-1} dz$$

Let $S_j^{[q]}$ be an eigenfunction of (6.1). This implies by definition of T_q that $S_j^{[q]}$ is an eigenfunction of T_q :

$$T_{q}S_{j}^{[q]} = (\Lambda_{j}^{[q]})^{-1}S_{j}^{[q]}.$$

We have then the following relation for the projection of an eigenfunction $S^{\left[q\right]}$ of T_{q} onto the eigenspace of T

(6.11)
$$S_{j}^{[q]} - E(\Lambda_{j}^{1})S_{j}^{[q]} = \frac{1}{2\pi i} \int_{\gamma} (T-zI)^{-1} (T_{q}-T) (T_{q}-zI)^{-1} S_{j}^{[q]} dz$$

In (6.8) the roles of T and T are reversed in comparison with [BO1], section 7.

Let us impose additional conditions on $S_{j,q}$:

Theorem 6.2. Let $S_{j+\ell}^{[q]} \ell = 0, \dots m(j)$ be the approximate (finite element) eigenfunctions associated with the eigenvalue Λ_j of multiplicity m(j) + 1. Then there exists $\bar{S}_{j+\ell,\,q} \in M(\Lambda_j)$ satisfying (3.4) such that

(6. 12)
$$\|\bar{\mathbf{S}}_{\mathbf{j}+\ell, \mathbf{q}} - \mathbf{S}_{\mathbf{j}+\ell}^{[\mathbf{q}]}\|_{\mathbf{E}(\Omega_{\mathbf{R}})} \le C\varepsilon_{\mathbf{j}}$$

(6.13)
$$\|\bar{\mathbf{S}}_{\mathbf{j}+\boldsymbol{\ell},\mathbf{q}} - \mathbf{E}(\mathbf{\Lambda}_{\mathbf{j}}^{-1})\mathbf{S}_{\mathbf{j}+\boldsymbol{\ell}}^{[\mathbf{q}]}\|_{\mathbf{E}(\Omega_{\mathbf{R}})} \le C\varepsilon_{\mathbf{j}}^{2}$$

where ε_i is defined by (6.5).

<u>Proof.</u> As mentioned previously, $E(\Lambda_j^{-1})S_{j+\ell}^{[q]}$ is the orthogonal projection of $S_{j+\ell}^{[q]}$ into $M(\Lambda_j)$. Let

(6.14)
$$\tilde{S}_{j+\ell, q} = E(\Lambda_{j}^{-1})S_{j+\ell}^{[q]}.$$

We have by orthogonality

(6.15)
$$\|S_{j+\ell}^{[q]}\|_{E(\Omega_R)}^2 - \|\widetilde{S}_{j+\ell,q}\|_{E(\Omega_R)}^2 = \|\widetilde{S}_{j+\ell,q} - S_{j+\ell}^{[q]}\|_{E(\Omega_R)}^2$$

and hence

$$(6.16) 0 \le 1 - \|\widetilde{S}_{j+\ell, q}\|_{E(\Omega_{R})}^{2} \le C\varepsilon_{j}^{2}.$$

Now we will construct by induction the orthonormal system of functions $\tilde{S}_{j+\ell,q}$, $\ell=0,\cdots,k$, satisfying (6.12) (6.13) by the Gram-Schmidt orthogonalization process. Assume now that (6.12) and (6.13) hold for $\ell=0,\cdots,\ k-1$ (for k=0 no assumption is necessary since $\hat{S}_{j+k,q}=\tilde{S}_{j+k,q}$ and only eq. (6.18), (6.21) below are used). Then we define

(6.17)
$$\hat{S}_{j+k,q} = \tilde{S}_{j+k,q} - \sum_{\ell=0}^{k-1} B_{\Omega_R} \left[\tilde{S}_{j+k,q}, \bar{S}_{j+\ell,q} \right] \bar{S}_{j+\ell,q}$$

and

(6.18)
$$\bar{S}_{j+k,q} = \frac{\hat{S}_{j+k,q}}{\|\hat{S}_{j+k,q}\|_{E(\Omega_R)}}.$$

Consider first

(6.19)
$$\hat{\hat{S}}_{j+k,q} = \tilde{S}_{j+k,q} - \sum_{\ell=0}^{k-1} B_{\Omega_R} \left[\tilde{S}_{j+k,q}, \tilde{S}_{j+\ell,q} \right] \bar{S}_{j+\ell,q}$$

Noting that by (6.14), (6.2a) we have

$$\begin{split} B_{\Omega_{R}} & \left[\tilde{S}_{j+k, q}, S_{j+\ell}^{[q]} - \tilde{S}_{j+\ell, q} \right] = 0, \quad k, \ell = 0, \cdots, m(j) \\ & B_{\Omega_{R}} \left[S_{j+k}^{[q]}, S_{j+\ell}^{[q]} \right] = 0, \quad k, \ell = 0, \cdots, m(j), \quad k \neq \ell \\ & B_{\Omega_{R}} \left[S_{j+k}^{[q]} - \tilde{S}_{j+k, q}, \tilde{S}_{j+\ell, q} \right] = 0, \quad k, \ell = 0, \cdots, m(j) \end{split}$$

and hence

$$\begin{split} &B_{\Omega_{R}}\left[\tilde{S}_{j+k,q},\tilde{S}_{j+\ell,q}\right] = \left[\tilde{S}_{j+k,q},S_{\ell}^{[q]}\right] \\ &= B_{\Omega_{R}}\left[\tilde{S}_{j+k,q} - S_{j+k}^{[q]},S_{j+\ell}^{[q]}\right] \\ &= B_{\Omega_{R}}\left[\tilde{S}_{j+k,q} - S_{j+k}^{[q]},S_{j+\ell}^{[q]} - \tilde{S}_{j+\ell,q}\right] . \end{split}$$

Therefore

$$|B_{\Omega_R}[\tilde{S}_{j+k,q},\tilde{S}_{j+\ell,q}]| \le C\varepsilon_j^2$$

This yields

$$\|\hat{\hat{S}}_{j+k,q} - \tilde{S}_{j+k,q}\|_{E(\Omega_R)} \le C\varepsilon_j^2$$

and by induction hypotheses we get also

(6.20)
$$\|\hat{\mathbf{S}}_{\mathbf{j}+\mathbf{k},\mathbf{q}} - \tilde{\mathbf{S}}_{\mathbf{j}+\mathbf{k},\mathbf{q}}\|_{\mathbf{E}(\Omega_{\mathbf{p}})} \le C\varepsilon_{\mathbf{j}}^{2}.$$

Using (6.16), we get

(6.21)
$$1 \ge \|\widetilde{S}_{j+k,q}\|_{E(\Omega_{\mathbb{P}})} \ge 1 - C\varepsilon_{j}^{2},$$

and from (6.20) we get

(6.22)
$$\left| \| \hat{\mathbf{S}}_{\mathbf{j}+\mathbf{k}, \mathbf{q}} \|_{\mathbf{E}(\Omega_{\mathbf{R}})} - 1 \right| \le C \varepsilon_{\mathbf{j}}^{2}.$$

Hence from (6.18) and (6.20) we get

$$\|\bar{S}_{j+k,q} - \tilde{S}_{j+k,q}\|_{E(\Omega_R)} \le C\varepsilon_j^2$$

which was to be proved.

7. Computation of the Vertex Intensity Factors

The exact value of the vertex intensity factor is given by (4.4). Hence we will numerically compute $C_j^{[q]}$ as follows:

(7.1)
$$C_{\mathbf{j}}^{[q]} = B_{\Omega_{\mathbf{R}}} \left[\mathbf{u}_{\mathbf{q}}, \mathbf{S}_{\mathbf{j}}^{[q]} \right] = \frac{\Lambda_{\mathbf{j}}^{[q]}}{R} \int_{\Gamma_{\mathbf{R}}^{0}} \mathbf{u}_{\mathbf{q}} \mathbf{S}_{\mathbf{j}}^{[q]} d\mathbf{s}.$$

We then want to estimate the error $C_{j}^{[q]} - C_{j}$.

As we said in the remark 4.1, the stress intensity factors C_j depend on the choice of exact eigenfunctions S_j . The eigenfunctions are not uniquely defined if the associated eigenvalue Λ_j is not simple. In this case we will consider the stress intensity factor $C_{j+\ell,q}$ which are associated with the eigenfunctions $\bar{S}_{j+\ell,q}$, $\ell=0,\cdots$ m, which were introduced in theorem 6.2. The decomposition (2.11a) of the exact solution can be expressed in this basis with vertex intensity factors $C_{j,q}$ depending on q:

$$u = u_0 + \sum_{\substack{j, +\frac{1}{2} \le s}} C_{j, q} \bar{S}_{j, q}.$$

For simplicity we will write in what follows S_j instead $\tilde{S}_{j,q}$. We have now

Theorem 7.1 Assume that the assumptions $A_1 - A_3$ are satisfied. Then for sufficiently large q we have

(7.2)
$$|C_{j}^{[q]} - C_{j,q}| \le C(F(N(q)))^{2}$$

Proof. Using (7.1) we have to show

$$|B_{\Omega_{\mathbf{R}}}\left[\mathbf{u}_{\mathbf{q}},\mathbf{S}_{\mathbf{j}}^{[\mathbf{q}]}\right] - B_{\Omega_{\mathbf{R}}}(\mathbf{u},\mathbf{S}_{\mathbf{j}})| \le C(F(N(\mathbf{q})))^{2}$$

We h

$$(7.4) B_{\Omega_{R}}\left(u_{q}, S_{j}^{[q]}\right) - B_{\Omega_{R}}(u, S_{j}) = B_{\Omega_{R}}(S_{j} - S_{j}^{[q]}, u) + B_{\Omega_{R}}(S_{j}, u - u_{q})$$

$$- B_{\Omega_{R}}\left(S_{j} - S_{j}^{[q]}, u - u_{q}\right) = D_{1} + D_{2} - D_{3}.$$

We will estimate D_{i} , i = 1, 2, 3 separately.

1) Estimate of D_3 . Using assumption A_3 , we get

$$|D_{3}| \le ||S_{j} - S_{j}^{[q]}||_{E(\Omega_{R})} ||u - u_{q}||_{E(\Omega_{R})} \le CF(N(q))^{2}$$

which follows immediately from (6.12).

2) Estimate of D_2 . Let $w \in H_D^1(\Omega)$ satisfy

$$(7.6) B_{\Omega}(w,v) = B_{\Omega_{R}}(S_{j},v) \ \forall v \in H_{D}^{1}(\Omega)$$

The function w exists and is unique. It can be readily seen that (7.6) is the variational formulation of the problem

$$\begin{cases}
\Delta w = 0 & \text{in } \Omega_{R} \\
\Delta w = 0 & \text{in } \Omega - \overline{\Omega}_{R} \\
w|_{\Gamma_{D}} = 0 & \frac{\partial w}{\partial n}|_{\Gamma_{N}} = 0 \\
[w]_{\Gamma_{R}^{\circ}} = 0 & \left[\frac{\partial w}{\partial n}\right]_{\Gamma_{R}^{\circ}} = \frac{\partial}{\partial n} S_{j}|_{\Gamma_{R}^{\circ}}
\end{cases}$$

By $[\cdot]_{\Gamma_{R}^{o}}$ we denoted the jump across Γ_{R}^{0} . Let $w_{1} = w|_{\Omega_{R}}$, $w_{2} = w|_{\Omega - \bar{\Omega}_{R}}$ and define \tilde{w}_{1} in Ω_{2R} by

$$(7.8) \qquad \tilde{w}_1 = \begin{cases} w_1 & \text{in } \Omega_R \\ w_2 - \frac{\Lambda_j}{1+2\Lambda_j} \left[S_j - R^{1+2\Lambda_j} S_{-j} \right] & \text{in } \Omega_{2R} - \bar{\Omega}_R \end{cases}.$$

Because we have $S_j = R^{1+2\Lambda_j}S_{-j}$ on Γ_R^0 , we have $[\tilde{w}_1]_{\Gamma_R^0} = 0$ and since

$$\frac{\partial}{\partial n} \left[S_j - R^{1+2\Lambda_j} S_{-j} \right] = \frac{2\Lambda_j + 1}{\Lambda_j} \frac{\partial S_j}{\partial n} \quad \text{we get} \quad \left[\frac{\partial}{\partial n} \; \widetilde{w}_i \right]_{\Gamma_R^0} = 0.$$

Further, $\Delta w_1 = 0$ on Ω_R and $\Delta w_2 = 0$ on $\Omega_{2R} - \overline{\Omega}_R$. Hence $\Delta \widetilde{w}_1 = 0 \text{ on } \Omega_{2R} \text{ and } \widetilde{w}_1 \in H^1_D(\Omega_{2R}).$ This shows that w can be analytically extended from Ω_R into Ω_{2R} as a harmonic function.

Analogousl, we can extend the function w_2 on $\Omega - \Omega_{R/2}$ by defining

(7.9)
$$\tilde{w}_{2} = \begin{cases} w_{2} & \text{in } \Omega - \Omega_{R} \\ w_{1} + \frac{\Lambda_{j}}{1+2\Lambda_{j}} \left[S_{j} - R^{1+2\Lambda_{j}} S_{-j} \right] & \text{in } \Omega_{R} - \bar{\Omega}_{R/2} \end{cases}$$

Because of (5.1) we have for any $w_q \in W_q(\Omega)$

$$D_2 = B_{\Omega_R}(S_j, u-u_q) = B(w, u-u_q) = B(w-w_q, u-u_q).$$

Using assumption A_2 we get

(7.10)
$$|D_{2}| \leq \inf_{\zeta \in W_{1}(\Omega)} ||w-\zeta||_{E(\Omega)} ||u-u_{q}||_{E(\Omega)} \leq CF(N(q))^{2}$$

3) Estimate of D_1 .

Define as in (6.14)

(7.11)
$$\tilde{S}_{j}^{[q]} = E(\Lambda_{j}^{-1})S_{j}^{[q]}.$$

Then

$$S_{j} - S_{j}^{[q]} = S_{j} - \tilde{S}_{j}^{[q]} + \tilde{S}_{j}^{[q]} - S_{j}^{[q]}$$

For sufficiently large q we have using (6.11)

$$S_{j}^{[q]} - \tilde{S}_{j}^{[q]} = S_{j}^{[q]} - E(\Lambda_{j}^{-1})S_{j}^{[q]} =$$

$$= \frac{1}{2\pi i} \int_{\chi} (T - zI)^{-1} (T_{q} - T) (T_{q} - zI)^{-1} S_{j}^{[q]} dz.$$

Since $T_q S_j^{[q]} = \frac{1}{\Lambda_j^{[q]}} S_j^{[q]}$ we have

$$(T_{q} - zI)^{-1}S_{j}^{[q]} = \frac{1}{(\Lambda_{j}^{[q]})^{-1}-z}S_{j}^{[q]}$$

and hence

$$\begin{split} B_{\Omega_{R}} \bigg[S_{\mathbf{j}}^{[q]} - \tilde{S}_{\mathbf{j}}^{[q]}, \mathbf{u} \bigg] &= \frac{1}{2\pi i} \int\limits_{\gamma} B_{\Omega_{R}} ((T-z\mathbf{I})^{-1} (T_{\mathbf{q}}-T) (T_{\mathbf{q}}-z\mathbf{I})^{-1} S_{\mathbf{j}}^{[q]}, \mathbf{u}) dz. \\ &= \frac{1}{2\pi i} \int\limits_{\gamma} B_{\Omega_{R}} \bigg[(T-z\mathbf{I})^{-1} (T_{\mathbf{q}}-T) \ \frac{1}{(\Lambda_{\mathbf{j}}^{[q]})^{-1}-z} \ S_{\mathbf{j}}^{[q]}, \mathbf{u} \bigg] dz. \end{split}$$

By (3.1) we have

$$\mathsf{B}_{\Omega_{\mathsf{R}}}(\mathsf{Tw},\mathsf{v}) \; = \; \mathsf{B}_{\Omega_{\mathsf{R}}}(\mathsf{w},\mathsf{Tv}) \,, \; \; \forall \mathsf{w},\mathsf{v} \in \mathsf{H}^1_\mathsf{D}(\Omega_{\mathsf{R}})$$

and hence

$$B_{\Omega_R}((T-zI)^{-1}w, v) = B_{\Omega_R}(w, (T-zI)^{-1}v)$$

which yields

$$B_{\Omega_{R}}\left[S_{j}^{[q]} - \tilde{S}_{j}^{[q]}, u\right] = \frac{1}{2\pi i} \int_{\pi} B_{\Omega_{R}}((T_{q} - T)((\Lambda_{j}^{[q]})^{-1} - z)^{-1} S_{j}^{[q]}, (T - zI)^{-1} u) dz.$$

Because $u|_{\Omega_R} \in \mathcal{L}(\Omega_R)$ we can write

(7.12)
$$u = \sum_{k=1}^{\infty} C_k S_k$$

$$(7.13) \sum_{k=1}^{\infty} |C_k|^2 < \infty.$$

Hence

$$(T-zI)^{-1}u = \sum_{k=1}^{\infty} (\Lambda_k^{-1}-z)^{-1}C_kS_k.$$

Let us define

(7.14)
$$\tilde{u} = \frac{1}{2\pi i} \int_{\gamma} \left[\left[\Lambda_{j}^{[q]} \right]^{-1} - z \right]^{-1} (T-z)^{-1} u \, dz$$

$$= \sum_{k=1}^{\infty} C_{k} S_{k} \int_{\gamma} \left[\left[\Lambda_{j}^{[q]} \right]^{-1} - z \right]^{-1} (\Lambda_{k}^{-1} - z)^{-1} dz.$$

Since $\Lambda_{j+\ell}^{-1} = \Lambda_{j}^{-1}$, $\ell = 1, \cdots, m(j)$ is inside of the circle γ and all other Λ_{k}^{-1} are outside we have from the residual theorem using the poles at $z = \Lambda_{k}^{-1}$ and $z = (\Lambda_{j}^{[q]})^{-1}$

$$\frac{1}{2\pi i} \int_{\gamma} \left[\left[A_{j}^{\left[q\right]} \right]^{-1} - z \right]^{-1} \left(A_{k}^{-1} - z \right)^{-1} dz$$

$$= \left\{ \begin{array}{ll} 0 & \text{for } k=j+\ell, \ \ell=0,\cdots,m(j) \\ \left[\left[\Lambda_{j}^{\left[q\right]}\right]^{-1} - \left[\Lambda_{k}^{-1}\right]^{-1}\right]^{-1} & \text{for } k\neq j+\ell, \ \ell=0,\cdots,m(j) \end{array} \right.$$

Therefore

(7.15)
$$\widetilde{\mathbf{u}} = \sum_{k=1}^{\infty} \left[\left(\Lambda_{\mathbf{j}}^{[q]} \right)^{-1} - \Lambda_{\mathbf{k}}^{-1} \right]^{-1} C_{\mathbf{k}} S_{\mathbf{k}}$$

$$\mathbf{x} \neq \mathbf{j} + \ell$$

and hence for any $\zeta \in H^1_D(\Omega_R)$

$$|B_{\Omega_{\mathbf{R}}}\left[\mathbf{S}_{\mathbf{j}+\boldsymbol{\ell}}^{[q]} - \tilde{\mathbf{S}}_{\mathbf{j}+\boldsymbol{\ell}}^{[q]}, \mathbf{u}\right]| = |B_{\Omega_{\mathbf{R}}}\left[(T_{\mathbf{q}} - T)\mathbf{S}_{\mathbf{j}+\boldsymbol{\ell}}^{[q]}, \tilde{\mathbf{u}}\right]|$$

$$= |B_{\Omega_{\mathbf{R}}}\left[(T_{\mathbf{q}} - T)\mathbf{S}_{\mathbf{j}+\boldsymbol{\ell}}^{[q]}, \tilde{\mathbf{u}} - \zeta\right]| \leq \|(T_{\mathbf{q}} - T)\mathbf{S}_{\mathbf{j}+\boldsymbol{\ell}}^{[q]}\|_{\mathbf{E}(\Omega_{\mathbf{R}})} \cdot \|\tilde{\mathbf{u}} - \zeta\|_{\mathbf{E}(\Omega_{\mathbf{R}})}.$$

Let us estimate both terms. To this end we write

$$(T_{q} - T)S_{j+\ell}^{[q]} = (T_{q} - T)S_{j+\ell} + (T_{q} - T)(S_{j+\ell}^{[q]} - S_{j+\ell})$$

and

$$(T_q - T)S_{j+\ell} = (\Pi_q^R - I)TS_{j+\ell} = (\Pi_q^R - I)\Lambda_j^{-1}S_{j+\ell}$$

Then using assumption A_3 we get

$$\|(T_{\mathbf{q}}^{-T})S_{\mathbf{j}+\boldsymbol{\ell}}\|_{\mathrm{E}(\Omega_{\mathbf{R}})} \leq C\Lambda_{\mathbf{j}}^{-1} \max_{\boldsymbol{\ell}=0,\cdots,m(\mathbf{j})} \|S_{\mathbf{j}+\boldsymbol{\ell}}^{-\zeta}\|_{\mathrm{E}(\Omega_{\mathbf{R}})} \leq CF(N(\mathbf{q})).$$

Further because $\|T_q^{-T}\|_{E(\Omega_R)\to E(\Omega_R)} \le 1$ (for q sufficiently large) we get

$$\| (T_{\mathbf{q}} - T) \left[\mathbf{S}_{\mathbf{j} + \ell}^{[\mathbf{q}]} - \mathbf{S}_{\mathbf{j} + \ell} \right] \|_{\mathbf{E}(\Omega_{\mathbf{R}})} \le \| \mathbf{S}_{\mathbf{j} + \ell}^{[\mathbf{q}]} - \mathbf{S}_{\mathbf{j} + \ell} \|_{\mathbf{E}(\Omega_{\mathbf{R}})} \le C(\mathbf{F}(\mathbf{N}(\mathbf{q}))).$$

and hence

(7.18)
$$\| (T_{q}^{-T})S_{j+\ell}^{[q]} \|_{E(\Omega_{R})} \leq CF(N(q)).$$

Let us now estimate the second term in (7.16).

We know that $u \in \mathcal{L}(\Omega_{2R})$. Hence $u^*(x) = u(2x) \in \mathcal{L}(\Omega_R)$. Therefore we can write

(7.19)
$$u^* = \sum_{k=1}^{\infty} C_k^* S_k$$

with

(7.20)
$$\sum_{k=1}^{\infty} |C_k^*|^2 < \infty.$$

On the other hand we have on $\Omega_{R/2}$.

(7.21)
$$u^{*}(x) = u(2x) = \sum_{k=1}^{\infty} C_{k} S_{k}(2x) = \sum_{k=1}^{\infty} C_{k} 2^{\Lambda_{k}} S_{k}(x)$$

and (7.19) yields

$$C_{\mathbf{k}}^{\bullet} = C_{\mathbf{k}} 2^{\Lambda_{\mathbf{k}}}$$

$$(7.23) \qquad \sum_{k=1}^{\infty} c_k^2 2^{2\Lambda_k} < \infty$$

Now we consider $\tilde{u}^*(x) = \tilde{u}(2x)$. We get from (7.15) for $x \in \Omega_R$

(7.24)
$$\tilde{u}^{*}(x) = \sum_{k=1}^{\infty} d_{k} S_{k}(x)$$

where

(7.25)
$$d_{k} = \begin{cases} \left[(\Lambda_{j}^{[q]})^{-1} - \Lambda_{k}^{-1} \right]^{-1} C_{k} 2^{\Lambda_{k}}, & k \neq j+\ell \\ 0 & k = j+\ell \end{cases}$$

Since for $k \neq j+\ell$ the numbers Λ_k^{-1} are outside of γ and $(\Lambda_{j+\ell}^{[q]})^{-1}$ is inside of γ (for q sufficiently large) we have

$$|\Lambda_{\mathbf{k}}^{-1} - \left[\Lambda_{\mathbf{j}}^{[q]}\right]^{-1}| \ge C_0 > 0.$$

(7.25), (7.26), (7.22), (7.23) yield

$$\sum_{k=1}^{\infty} (d_k)^2 \le \frac{1}{C_0^2} \sum_{k=1}^{\infty} |C_k^*|^2 < \infty$$

Therefore $\tilde{u}^* \in \mathcal{L}(\Omega_R)$ and hence $\tilde{u} \in \mathcal{L}(\Omega_{2R})$. Using assumption A_3 we have

(7.27)
$$\inf_{\zeta \in W_{\mathbf{q}}(\Omega_{\mathbf{R}})} \|\widetilde{\mathbf{u}} - \zeta\|_{\mathbf{E}(\Omega_{\mathbf{R}})} \leq CF(\mathbf{N}(\mathbf{q})).$$

Hence from (7.16) using (7.18) and (7.27)

(7.28)
$$\left| B_{\Omega_{R}} \left[S_{j+\ell}^{[q]} - \tilde{S}_{j+\ell}^{[q]}, u \right] \right| \leq CF(N(q))^{2}$$

Using now (6.13) we get

$$\left| B_{\Omega_{\mathbf{R}}} \left[\mathbf{S}_{\mathbf{j}+\boldsymbol{\ell}}^{[q]} - \mathbf{S}_{\mathbf{j}+\boldsymbol{\ell}}, \mathbf{u} \right] \right| \leq CF(N(q))^{2}$$

i.e. $|D_1| \le CF(N(q))^2$ what was to be proven.

Remark 7.1 We have assumed that (2.6) holds. This allows us to use the decomposition (2.11). In the general case the decomposition is more complex. The present theory can be generalized to this case but we will not address the problem here.

8. Numerical Results

Let us consider the following mixed boundary value problem. Let $\,\Omega\,$ be a cube with a crack,

$$\Omega = \{|x_j| < 1, \ j = 1, 2, 3\} - \{(x_1, x_2, 0) | 0 \le x_1 \le 1, \ 0 \le x_2 \le 1\}$$
 as shown in Fig. 8.1.

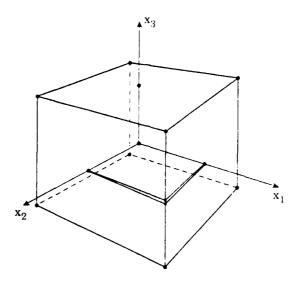


Figure 8.1. The cracked cube

On both sides of the crack and the two faces $x_1 = 1$ and $x_2 = 1$ Dirichlet conditions u = 0 are prescribed. On the remaining 4 faces of the cube the following Neumann conditions are prescribed

i)
$$\frac{\partial u}{\partial n} = 0$$
 on the faces $x_1 = -1, x_2 = -1$

ii)
$$\frac{\partial u}{\partial n} = \cos \frac{\pi}{4} (x_1 + 1) \cos \frac{\pi}{4} (x_2 + 1) \quad \text{for} \quad x_3 = \pm 1$$

The boundary conditions imply that the solution will not have singularities at the edges and vertices of the cube (since one can use even and odd extensions). The solution has a singularity at the two edges of the cracks, $(0,1) \times \{0\} \times \{0\}$ and $\{0\} \times (0,1) \times \{0\}$ and at the vertex at (0,0,0). For a more detailed description of the edge and vertex singularities in this

example see [PS1]. The (smallest) leading edge singularity exponent is $\alpha=\frac{1}{2}$. The leading vertex singularity exponent Λ_1 is not analytically known, our computational results below show $\Lambda_1\approx 0.2966$. We use symmetry and analyze only the half cube $(-1< x_3<0)$ computationally. The p-version of the finite element method implemented in the program STRIPE [S] is used. We used two different meshes, the "unrefined mesh" and the "refined mesh." Both meshes contain a ball around the vertex at 0.

Figure 8.2 shows the unrefined mesh. For clarity, the mesh inside $\,\Omega_{R}^{}$ is shown separately.

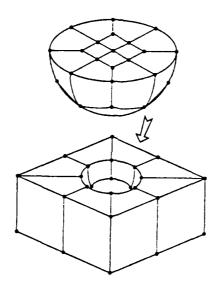


Figure 8.2. The basic unrefined mesh around the vertex at 0.

In Figure 8.3 we show the refined (geometrical) mesh with 6 layers. The sizes of adjoining layers have a ratio of $\sigma = 0.15$ for the mesh used in the computation (in Fig. 8.3 $\sigma = 0.5$ is used for clarity).

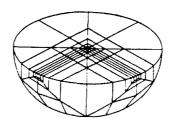


Figure 8.3. Detail of the geometrically refined mesh in the neighborhood of the vertex at 0.

In table 8.1 we report N(q) and the computed values of $\Lambda_1^{[q]}$, $C^{[q]}$ and $\|u_q\|_{E(\Omega)}^2$ for the mesh shown in Figure 8.2 as function of the degree p of the elements. Table 8.2 gives analogous results for the refined mesh (with 6 layers) shown in Figure 8.2. From tables 8.1 and 8.2 we clearly see the effect of the refinement of the mesh. By using a more refined mesh, a higher value of p and extrapolation, we estimate the exact values for $\|u\|_{E(\Omega)}^2$, Λ_1 , C_1 as

(8.1)
$$\Lambda_1 = 0.29658 \quad C_1 = 10.123, \quad \|\mathbf{u}\|_{E(\Omega)}^2 = 8.66908$$

Table 8.1. The values of Λ_1, C_1 and $\|\mathbf{u}\|_{E(\Omega)}^2$ for the mesh shown in Fig. 8.2

P	N	^ [q]	C[q]	∥u∥ ² E(Ω)	
2	133	0.315743	9,50571	8.5697572	
3	231	0.313768	9.55731	8.5867675	
4	420	0.307749	9.75874	8.6263436	
5	700	0.304403	9.86982	8.6403593	
6	1099	0.302277	9.93970	8.6485159	
7	1645	0.300888	9.98514	8.6536345	
8	2366	0.299943	10.0161	8.6570896	
9	3290	0.299274	10.0380	8.6595274	
10	4445	0.298785	10.0540	8.6613051	
11	5859	0.298418	10.0660	8.6626398	

Table 8.2. The values of Λ_1, C_1 and $\|u\|_{E(\Omega)}^2$ for the refined mesh shown in Fig. 8.2

P	N	Λ ^[q]	C[q]	$\ \mathbf{u}\ _{E(\Omega)}^2$
2	1438	0.297669	10.5183	8.6049893
3	2582	0.296866	10.1308	8.6320936
4	4852	0.296603	10.1317	8.6671875
5	8304	0.296589	10.1210	8.6686951
6	13326	0.296584	10.1214	8.6690024

We use the values on (8.1) to compute the relative errors

$$\frac{\|\mathbf{u}_{\mathbf{q}} - \mathbf{u}\|_{\mathbf{E}}^{2}}{\|\mathbf{u}\|_{\mathbf{F}}^{2}}, \frac{\|\mathbf{\Lambda}_{1}^{[\mathbf{q}]} - \mathbf{\Lambda}_{1}\|}{\|\mathbf{\Lambda}_{1}\|}, \frac{\|\mathbf{C}_{1}^{[\mathbf{q}]} - \mathbf{C}_{1}\|}{\|\mathbf{C}_{1}\|}.$$

In Figure 8.4 we show these relative errors for the mesh shown in Figure 2. We see that the errors of C_1 and Λ_1 decrease with the same rate as the square of the error in the energy norm as predicted by theorems 6.1, 7.1. We obtain from estimates (5.7) (5.8) that the error behaves like $O((N(q))^{-2/3})$. This rate is indicated in Figure 8.4 too. We see that the asymptotic analysis of previous section is completely applicable in the computed range.

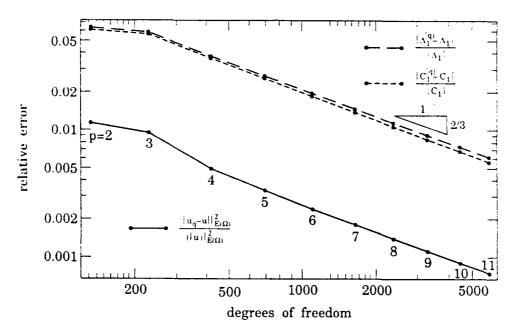


Figure 8.4 Relative error for unrefined mesh

In Figure 8.5 we show analogous results for the refined mesh. We see that also here the accuracy of Λ_1 and C_1 increases as the square of the error measured in the energy norm. We are in the preasymptotic range of the p-version, which can be interpreted as the h-p version. For large p, the errors again decrease with the rate $O(N(q)^{-2/3})$. The corresponding slope is indicated in Fig. 8.5.

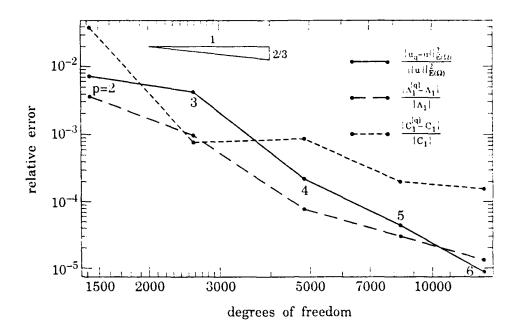


Figure 8.5 Relative error for the mesh with geometric refinement

We note that we have used here the classical p-version with the same degree p of polynomials in all elements. By using low values of p close to singularities and high values of p away from the singularities comparable results can be obtained with a much smaller number of degrees of freedom.

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